Lawrence Livermore National Laboratory

October/November 2013

Science & Technology REVIEW

2013

Livermore Wins 5 R&D 100 Awards

2013 R&D 100

Also in this issue:

Collaborative Earthquake Exhibit Debuts

Modeling the Nuclear Weapons Enterprise

About the Cover

Laboratory researchers captured five R&D 100 awards in *R&D Magazine*'s annual competition for the top 100 industrial innovations worldwide. Highlights beginning on p. 4 describe the award-winning technologies: DNA-tagged reagents for aerosol experiments, efficient mode converters for high-power fiber amplifiers, movie-mode dynamic transmission electron microscopy, a high-throughput screening tool for identifying energetic laser distortion, and a collection of software prototypes (mini-apps) that allow developers to measure the performance of new computing environments. Since 1978, Livermore researchers have received 148 R&D 100 awards. The R&D 100 logo is reprinted in this issue courtesy of *R&D Magazine*.

Cover design: Amy E. Henke

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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2013 R&D 100 Awards

Research Highlights

Departments

Nation's Renewable Energy Use on the Rise

Each year, the Laboratory releases flowcharts that track the nation's consumption of energy resources. According to the most recent U.S. charts released, Americans used less coal and more natural gas, solar panels, and wind turbines to generate electricity in 2012 (flowcharts.llnl.gov).

"Natural gas use is up particularly in the electricity generation sector," says A. J. Simon, a Livermore energy systems analyst. Sustained, low natural-gas prices have prompted a shift from coal to gas in this sector. According to Simon, the rise in renewables is tied to prices (the underlying cost of solar panels and wind turbines has gone down) and policy (government incentives to equipment installers as well as renewable energy targets in various states). Overall, Americans used 2.2 quadrillion British thermal units, or quads, less coal in 2012 than the previous year, while natural gas use jumped to 26 quads from 24.9 quads the previous year.

Once again, wind power saw the highest percentage gains, from 1.17 quads produced in 2011 to 1.36 quads in 2012. In response to government-sponsored incentives to invest in renewable energy, new wind farms continue to come online with larger, more efficient turbines than have been previously developed. Solar also jumped from 0.158 quads in 2011 to 0.235 quads in 2012. Extraordinary declines in the price of photovoltaic panels because of global oversupply drove this shift.

"This year is the first in at least a decade that we've seen a measurable decrease in nuclear energy," says Simon. "The cut is likely permanent because four nuclear reactors recently went offline. A couple of nuclear plants are under construction, but they won't come online for another few years."

The majority of energy use in 2012 was for electricity generation (38.1 quads), followed by the transportation, industrial, residential, and commercial sectors. However, energy use in the residential, commercial, and transportation sectors decreased while industrial energy use increased slightly.

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Record Pressure for Solid Iron Achieved

In a series of experimental campaigns led by Livermore's Yuan Ping using the OMEGA laser at the University of Rochester's Laboratory for Laser Energetics (LLE), researchers compressed iron up to 5.6 million atmospheres (5.6 million times the pressure at Earth's surface), a record for solid iron. Iron is the most abundant element in Earth's core and the sixth most abundant element in the universe. As a key component of terrestrial planets and exoplanets, it is one of the materials most often studied under extreme conditions.

The record pressure was achieved using multishock compression. A series of shocks (rather than a single shock) keeps the entropy low during material compression, which is key to maintaining the temperature lower than iron's melting point and allowing it to remain solid. The team used an x-ray technique called EXAFS (extended x-ray absorption fine structure) to diagnose iron's material properties under the extreme pressure. This effort resulted in the first EXAFS data in high-energy-density (HED) matter.

The data show that the close-packed structure of iron is stable in the regime explored, confirming simulation predictions and experimental studies using x-ray diffraction up to 3 million atmospheres. Unexpectedly, the team found that the temperature at peak compression is significantly higher than that from pure compressive work, and the dynamic strength of iron is many times greater than the static strength based on lower pressure data.

Ping says, "The measurement technique can now be scaled up to larger laser systems, such as the National Ignition Facility, to reach higher pressures or to study dynamics in HED materials." The research was reported in the August 9, 2013, issue of *Physical Review Letters*. The work was funded by the Laboratory Directed Research and Development Program and the Department of Energy's HED Laboratory Plasmas Program. Livermore coauthors are Federica Coppari, Damien Hicks, Dayne Fratanduono, Sebastien Hamel, Jon Eggert, James Rygg, Raymond Smith, Damian Swift, David Braun, and Gilbert Collins. The team also includes two coauthors from LLE, Barukh Yaakobi and Tom Boehly.

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(*continued on p. 24*)

Commentary by A. J. Simon

Diversity of Science Addresses Broad Missions

As this year's scientific editor of *Science & Technology Review* (*S&TR*), I have been tasked with exploring the remarkable diversity of research being undertaken at Lawrence Livermore. My assignment has afforded me the opportunity to learn what our researchers are doing and why. It has been a yearlong immersion with extraordinary technical experts, who are just as passionate about making the world a safer place as they are about pursuing scientific research.

This diversity, of both science and the national mission it supports, is on display in this issue of *S&TR*, which features the Laboratory's R&D 100 Award winners for 2013. Each year, *R&D Magazine* presents these "Oscars of Innovation" to the top 100 technological advances that contribute to meeting an important national or societal need. Livermore garnered five awards in 2013, bringing the Laboratory's total to 148 since 1978. The highlights beginning on p. 4 showcase the winning technologies: DNA-tagged reagents for aerosol experiments, efficient mode converters for high-power fiber amplifiers, movie-mode dynamic transmission electron microscopy, a high-throughput screening tool for identifying energetic laser distortion, and a collection of software proxies (mini-apps) that allow developers to measure the performance of new computing environments. The development teams included computer scientists, electrical and optical engineers, laser scientists, biologists, material scientists, and electron microscopists, who together worked to find innovative solutions for various government agencies: the National Nuclear Security Administration, Department of Homeland Security, Department of Energy's Office of Science, and Department of Defense.

The intellectual range and applicability of the Laboratory's work are further exemplified by two other stories in this issue: enterprise modeling (p. 19) and seismic simulation (p. 14). These projects effectively span the Laboratory's mission scope—from support for decision making to sustain our nation's strategic deterrent, to application of the Laboratory's capabilities for enhancing science education in our local community.

Livermore's work in systems analysis and optimization science are an integral part of our nation's planning for how to maintain an effective nuclear weapons enterprise in a rapidly changing global environment. This mathematically demanding work depends on the application of expertise, detailed knowledge, and copious data gathered from across the enterprise. The data pertain to the nation's weapons, facilities, and personnel as well as the dynamic interactions of system components. A team of analysts and engineers has risen to meet the challenge, delivering computer models and analysis products to personnel in the departments of Energy and Defense whose enduring mission is nuclear deterrence.

At the other end of the spectrum, the collaboration between a team of Livermore seismologists and the California Academy of Sciences illustrates how high-fidelity seismic data can be rendered into animations that both inform and entertain the general public. Since the Laboratory's inception in 1952, education and public outreach have been essential ingredients in our culture and mission responsibility. Therefore, distilling the complexity of a global, three-dimensional seismic-wave propagation simulation into an IMAX movie was a natural step for the Livermore team. The results are spectacular: the production team at the Academy stitched gigabytes of data from two separate simulations into a single shot that renders earthquake physics at multiple scales into a scene that is technically accurate, but accessible to the general public.

By developing a completely different but no less impressive movie-making technology, a team from Livermore has won an R&D 100 Award for the movie-mode dynamic transmission electron microscope (MM-DTEM). (See p. 8 and *S&TR*, September 2013, pp. 4–11.) With a combination of precision lasers, an ultrahigh-resolution microscope, and sophisticated electron-beam optics, MM-DTEM captures video of previously unseen fleeting phenomena at the nanometer scale. This sophisticated instrument enables the intuitive understanding of complex natural systems that can only be achieved by direct observation.

The Laboratory addresses global, national, and local security challenges, through interdisciplinary teams of scientists and engineers. As individual experts, we are immersed in a community of technical knowledge, exchanging ideas with colleagues who are also expert in a multitude of other fields. As teams, we systematically eliminate the unknown and achieve what was thought to be impossible. Exploring the interests and accomplishments of my colleagues could satisfy the most voracious scientific curiosity. It has truly been a pleasure to work with the staff of *S&TR*, helping to bring these diverse stories to life.

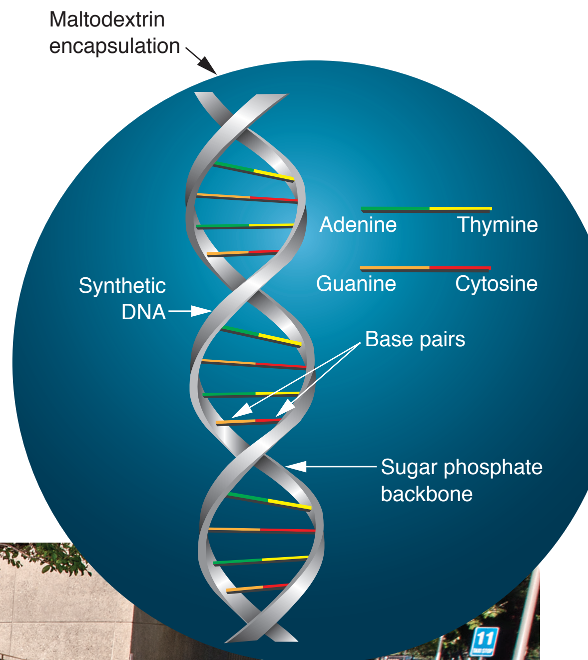
■ A. J. Simon is the 2013 scientific editor of *Science & Technology Review.*

DNA-Tagged Sugar Particles Simulate Aerosol Airflow Patterns

CHEMICALS, mold, and biological pathogens are often common constituents of the air we breathe at the home or office, in public places such as subway stations and restaurants, and on airplanes. Indeed, one of the most overlooked threats to human health is poor indoor air quality, often termed "sick building syndrome." Experts have long searched for a safe and reliable method to improve understanding of airflow and the transport of airborne particles.

In response to this pressing need, a team of Livermore scientists and engineers has developed a safe and versatile technology for tracking airflow called DNA-tagged reagents for aerosol experiments (DNATrax). The DNATrax development effort, funded

Microparticles used in DNA-tagged reagents for aerosol experiments (DNATrax) are composed of sugars approved by the Federal Drug Administration for food production.



Livermore development team for DNATrax: (from left) Roald Leif, Ruth Udey, Sally Hall, Elizabeth Wheeler, George Farquar, and Brian Baker. (Not shown: Christine Hara, Maxim Shusteff, Cindy Thomas, and Beth Vitalis.)

by the U.S. Defense Threat Reduction Agency, was led by physical chemist George Farquar. The patented technology combines Federal Drug Administration– (FDA-) approved foodstuffs, such as sugar, and a unique DNA bar code to produce microparticles that can be used to track and quantify airflow in both indoor and outdoor venues. Potential applications include indoor air-quality detection for homes, offices, ships, and airplanes; urban particulate tracking for airports, convention centers, and subway and train stations; and tracking of environmental releases such as carbon dioxide. DNATrax, an R&D 100 Award–winning technology, is the first rapid and safe method to simulate aerosol particles that are easily inhaled.

Indoor air pollutants can include biological agents such as molds, bacteria, viruses, pollen, animal dander, and dust mites. Other common pollutants are sources of combustion products, such as tobacco smoke and wood-burning stoves, and chemicals used to manufacture building materials and household products, such as formaldehyde and asbestos. All of these contaminants "pool" in spaces having inadequate ventilation, with detrimental effects to building occupants. "Without adequate airflow, harmful pollutants can become concentrated and make us sick," says Farquar.

Pinpointing the areas where pollutants stagnate requires knowing how air flows in a given space. With this knowledge, airflow patterns could be adjusted to help improve building occupants' comfort and health. In addition, this knowledge could be used to strengthen chemical and biological defenses in buildings and ships by optimizing the locations of specialized detectors.

Successful Tests at the Pentagon

DNATrax offers a cost-effective and environmentally friendly diagnostic tool that can simulate a wide variety of aerosols. The technology has been used to model airflow in several enclosed spaces. In November 2012, a series of tests was successfully conducted at the Pentagon in conjunction with the Pentagon Force Protection Agency. Sets of different microparticles, each with a unique DNA segment (or bar code), were released in corridors and detected by both Pentagon and Livermore detectors. The tests enhanced the team's understanding of indoor airflow created by heating, ventilation, and air-conditioning systems.

DNATrax microparticles are produced by combining FDA-approved DNA bar-coded material in an aqueous solution. (See the figure on p. 4.) The mixture is then formed into droplets using either a modified ink-jet printer or a spray dryer. The resulting dried particles measure from 1 to 10 micrometers in diameter. The particle size can be adjusted for a particular application (to simulate a selected pathogen, for example) by changing the composition of the solution.

The bar codes comprise about 100 DNA bases of synthetically produced nucleic acid copied from genes unique to a deep-sea organism. The particular sequence of DNA bases can be varied to create a nearly unlimited variety of test particles. This organism was chosen because its DNA would be extremely unlikely to be detected in an office environment. The concentration of DNA used ensures that one or two copies are present in each microparticle. Particles may also be mixed with fluorophores that fluoresce under certain wavelengths of light.

Once an aerosol generator releases DNATrax microparticles, they can travel tens of meters depending on their size. The microparticles are collected by swipes or air filters and detected and counted using polymerase chain reaction (PCR) technology, or in the case of particles containing fluorophores, fluorescence particle spectroscopy.

No Decontamination Necessary

Farquar notes that other products on the market for tracking airflow, such as natural and genetically modified spores, can be expensive. They can also face significant regulatory and public perception barriers before being released in public places. Furthermore, once released, these spores must be removed, making the release site temporarily unavailable and limiting additional testing. Full decontamination can take days to complete. In contrast, DNATrax particles are biodegradable and nontoxic.

DNATrax also allows for simultaneous or repeated releases in a short time, which sharply reduces the costs associated with conducting tests. Several particle varieties can be released in a facility at the same time and still be identified through their DNA bar codes. No decontamination between releases is needed. In 2012, two different bar-coded particles were simultaneously released from neighboring locations. Using PCR, the two types of particles were easily differentiated, and their concentrations were measured as a function of the distance from their respective release points.

Farquar predicts DNATrax will revolutionize the science of detecting and tracking the flow of particulates and airborne contaminants. In addition, the novel, safe, and cost-effective technology should lead to advances in biology, environmental science, and fluid dynamics.

—Arnie Heller

Key Words: air quality, DNA-tagged reagents for aerosol experiments (DNATrax), pathogen, polymerase chain reaction (PCR), R&D 100 Award.

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Fiber Lasers Get a Power Boost

FIBER lasers are powerhouses in the laser field and used for many applications such as industrial machining. Although a fiber laser is capable of producing kilowatts of power, it is ultimately limited by the intense laser light damaging the fiber. Six Laboratory physicists—Arun Sridharan, John Heebner, Paul Pax, Derrek Reggie Drachenberg, James Armstrong, and Jay Dawson—came up with an R&D 100 Award–winning solution to this problem: efficient mode converters for high-power fiber amplifiers.

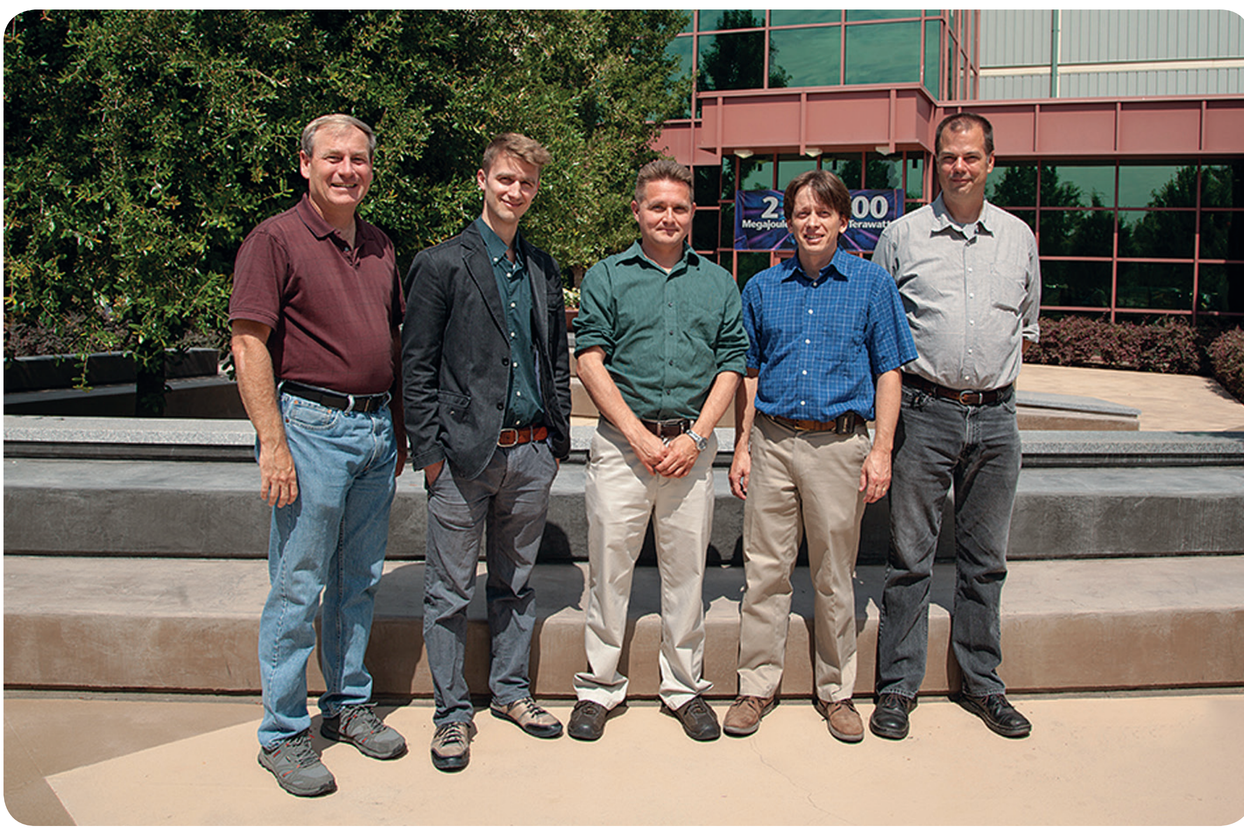
In the team's system, one mode converter takes light from a traditional circular-core fiber and reformats it geometrically for injection into a Livermore-designed ribbon-fiber amplifier with a wide, rectangular core. (See *S&TR*, June 2011, pp. 16–18; April/May 2013, pp. 12–15.) A second converter located beyond the ribbon-fiber amplifier reformats the high-power output into a beam that is optimized for delivery to the target. This technology can potentially scale the power of fiber lasers from a few kilowatts to 100 kilowatts, while maintaining high beam quality.

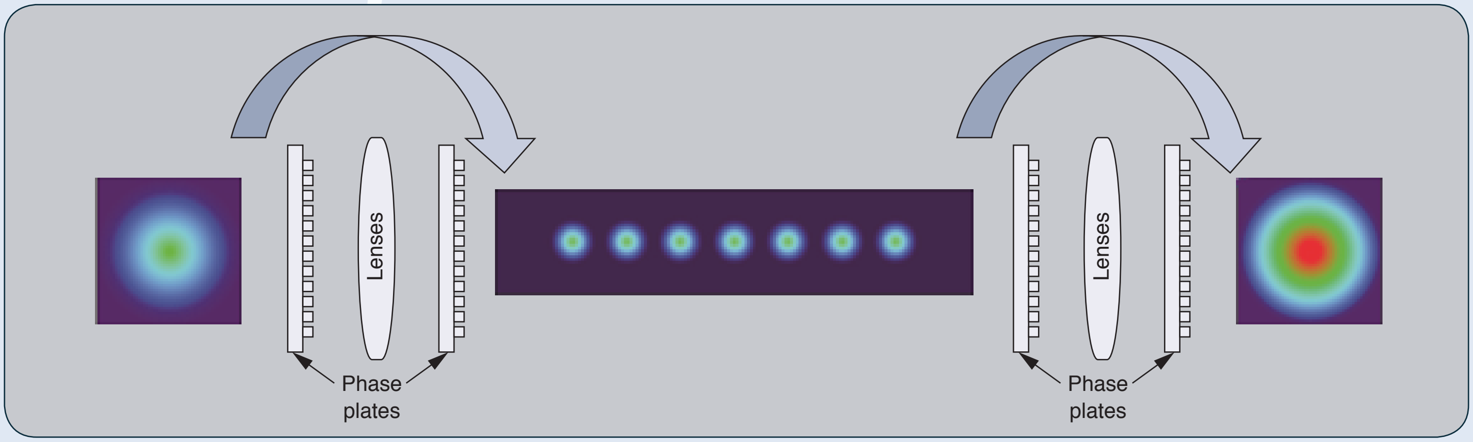
A Shape-Shifting Solution

A fiber laser is typically constructed of an optical fiber doped with rare-earth elements such as erbium, ytterbium, and neodymium. Traditional fiber lasers and amplifiers are robust, compact, efficient, and reliable. Because of their inherent flexibility, they can readily deliver output to a movable focusing element—an important requirement for high-precision laser cutting and other applications. They can also be amplified to kilowatt levels of continuous output power, because the fiber has a high surface area to volume ratio. Commercial single-mode lasers are capable of reaching 10 kilowatts.

However, power amplification in these lasers is limited. Heebner explains, "We could increase the average power by combining multiple lasers. But, to maintain the tight focus at a distance, we

Development team for the mode converter system: (from left) Jay Dawson, Derrek Reggie Drachenberg, John Heebner, James Paul Armstrong, and Paul Pax. (Not shown: Arun Sridharan.)





Key to the Livermore-developed mode converter system are the diffractive optical elements or "phase plates." Each glass phase plate has an active area of approximately 1 square centimeter. The two phase plates at left, in combination with multiple lenses, convert low-power laser light (about 10 micrometers in diameter, shown here head-on) from a circular-core fiber to a form that is easily coupled into and amplified by a rectangular "ribbon" fiber (about 10 by 100 micrometers, also shown head-on). A second set of phase plates located beyond the ribbon-fiber amplifier reformats the high-power output into a beam that is optimized for target delivery. The mode converter system fits easily on a tabletop.

need the laser to operate in a single-mode, diffraction-limited configuration. In this configuration, the laser light can be amplified only so much before it damages the fiber. Our approach to increasing the energy output past this damage threshold is to spread the laser power over a larger area in the fiber."

To obtain the larger area, the team moved from the traditional circular-core fiber amplifier to one with a rectangular core. The rectangular-core fiber allows the energy to spread over several peaks instead of being concentrated into the single peak of a circular-core, single-mode fiber.

"With the power distributed over many peaks or 'lobes,' we can amplify the laser light to a higher overall power without damaging the fiber," says Heebner. The technology behind this operation is a mode converter. The converter modifies the single-mode laser light, while maintaining its beam quality, to a high-order mode that can be amplified to much higher power levels. The device makes this conversion with the help of two diffractive optical elements known as phase plates. (See the figure above.) The first plate takes the incoming light's power distribution—often shaped with a Gaussian profile—and redistributes the power into multiple lobes that are appropriately matched to excite one of the ribbon-fiber modes. The second phase plate impresses the required phase to correct the wavefront of the distribution, yielding the alternating sign of the multiple lobes. Once the light is in the multiple-lobe configuration in the ribbon fiber, it can be safely amplified without destroying the fiber.

Finally, the now-amplified light passes through another pair of phase plates, similar to the first pair. These phase plates convert the multiple-lobe, high-order mode light back into a single-lobe, low-order mode that is better suited for projecting and focusing on a target. The mode converter system accomplishes these tasks with more than 80 percent efficiency, far higher than any other approach. "In addition to being very efficient," says Heebner, "our mode converter is simple, compact, and low cost."

Increased Power Benefits Defense and Manufacturing

Fiber-laser applications typically require a lot of power—tens of kilowatts—all focused on a target that is a considerable distance from the source. With the Livermore-developed mode converter system, fiber lasers for national defense and industrial-machining applications could generate 7 to 10 times the average power of traditional fiber lasers over longer distances.

In addition, the mode converters could be incorporated with slab, rod, and gas lasers, which are typically used in industrial machining. "We foresee an even wider base of applications beyond our initial focus," says Heebner. "We expect our mode converters to be of interest throughout industry and the departments of Energy and Defense."

—Ann Parker

Key Words: circular-core fiber, fiber laser, industrial laser, mode converter, R&D 100 Award, ribbon fiber.

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High-Speed Movies at the Nanoscale

CONVENTIONAL transmission electron microscopy is an extremely powerful tool for revealing the structure and properties of materials at atomic, nanometer, and micrometer scales; nonetheless, the tool has its limitations. For instance, transmission electron microscopy is not fast enough to measure rapidly evolving nano- and microscale processes that occur over very short timescales.

With the R&D 100 Award–winning movie-mode dynamic transmission electron microscope (MM-DTEM), scientists can now capture a sequence of nine images or diffraction patterns over a period of 1 to 100 microseconds. The resulting nine-frame movies provide details never before seen of basic material and biological processes, enabling an entirely new class of experiments and dynamic measurements.

Window to the World of the Very Small

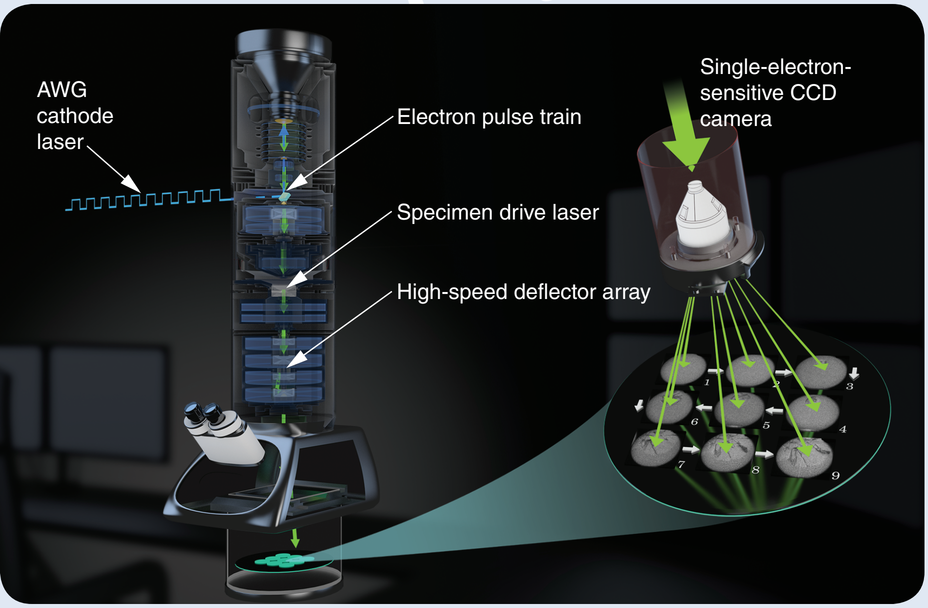
The Livermore MM-DTEM team led by Thomas LaGrange and Bryan Reed also includes Glenn Huete, Richard Shuttlesworth, and William DeHope. The product is marketed through Integrated Dynamic Electron Solutions, Inc., which also markets a product based on the precursor system called the single-shot DTEM. This earlier microscope, which won an R&D 100 Award in 2008, captures a single snapshot of a rapid process with nanosecond exposure times. (See *S&TR*, October/November 2008, pp. 4–5.) MM-DTEM changed the game with its ability to record multiple images of a fast-evolving material process. The product is ideally suited for directly observing complex processes such as microstructural changes, phase transformations, and chemical reactions. "These are the processes that govern the fabrication and real-world performance of nanostructured materials," says LaGrange.

The product could also be used to analyze little-understood biological processes, including host–pathogen interactions and protein–protein binding. For instance, MM-DTEM could capture conformational changes in molecules during the protein-binding process, allowing researchers to see how protein molecular structure evolves during binding, a process critical to biological function. (See *S&TR*, September 2013, pp. 4–11 for early applications of MM-DTEM.)

Lights, Camera, Action!

MM-DTEM is based on a transmission electron microscope modified to include two pulsed lasers—a sample drive laser and an arbitrary waveform generation (AWG) cathode laser.

The MM-DTEM development team: (from left) Thomas LaGrange, Glenn Huete, William DeHope, Richard Shuttlesworth, and Bryan Reed.



With the movie-mode dynamic transmission electron microscope (MM-DTEM), researchers can now capture the details of material processes that evolve over nanosecond timescales. This artist's conception of MM-DTEM shows the arbitrary waveform generator (AWG) cathode laser that produces precisely shaped and timed electron pulses, the high-speed pulse deflector that is synchronized with the AWG laser, and the high-resolution charge-coupled-device (CCD) camera that records the resulting array of images or diffraction patterns.

(See the figure above.) The sample drive laser releases a short (about 12-nanosecond-long) pulse that heats a small region of the specimen, initiating a desired process.

After an electronically controlled time delay, the AWG cathode laser emits a train of precisely shaped laser pulses. Each pulse strikes a photocathode, creating, in turn, an electron pulse with the same temporal shape as the initiating laser pulse. This AWG cathode laser is the heart of the system's innovation, providing a flexible platform that can create electron pulses lasting from 10 nanoseconds to 1 microsecond, and frame-to-frame spacing ranging from 50 nanoseconds to 150 microseconds.

Each electron pulse is then accelerated to 70 percent the speed of light and focused onto a specimen that is 5 to 250 nanometers thick. The electrons interact and pass through the material to lenses, which produce either diffraction patterns or real-space photographic images on a charge-coupled-device camera. A high-speed deflector array, precisely synchronized with the AWG cathode laser, deflects each pulse to a different region on the camera. The end result is a series of images that form the frames for a movie. The current system uses a 3-by-3 image array with 150-nanosecond frame-to-frame times and exposure intervals as short as 10 nanoseconds.

The team plans to expand the system's capabilities. For instance, with only minor upgrades, the system could produce a 5-by-5 array and take movies with even shorter interframe times. A new camera system under consideration would supply images of even higher resolution. "We're looking at using a direct-electron-detection camera, which would not depend on scintillators, is less noisy, and is more sensitive by a factor of 10," says LaGrange. "Because this camera records electrons directly, we would be able to use a lower-dose electron beam, which is preferable for imaging biological samples."

The team is also developing methods for exploring different processes in a variety of environments. "Heat from a laser pulse isn't the only way to initiate a process," says Reed. "For example, microelectromechanical system devices can rapidly apply high stress to a sample, deforming it. We could then examine high strain-rate deformation, defect formation, and other interactions that lead to material failure."

It's a Wrap

With frame rates over 100,000 times faster than those of conventional techniques, MM-DTEM is the only system that captures the fine-scale details of rapidly evolving nano- and microscale processes, for both organic and inorganic specimens. "With MM-DTEM, we're opening a new window to the world of small-scale, rapid processes," says LaGrange. "For the first time, researchers will be able to capture a tremendous range of fundamentally and technologically important processes and see the crucial in-between moments of material dynamics."

With the tiny worlds of nanomaterials looming larger in importance every day, tools are needed to record objects and structures at this level as they form, move, and interact. MM-DTEM now makes this nanoscale movie-making a reality.

—Ann Parker

Key Words: arbitrary waveform generator (AWG) cathode laser, electron pulse train, movie-mode dynamic transmission electron microscope (MM-DTEM), R&D 100 Award.

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Shielding the World's Largest Laser from Harmful Pulses

OPERATING the National Ignition Facility (NIF) presents many challenges, not the least of which is maintaining safe operating conditions for expensive laser amplifiers, mirrors, and other optical devices. The process of screening energetic laser pulses to avoid harming optics has often taken up to a day. As NIF evolves into a more dynamic facility with added flexibility in laser power and operating wavelength, reducing the time needed to screen these pulses is critical.

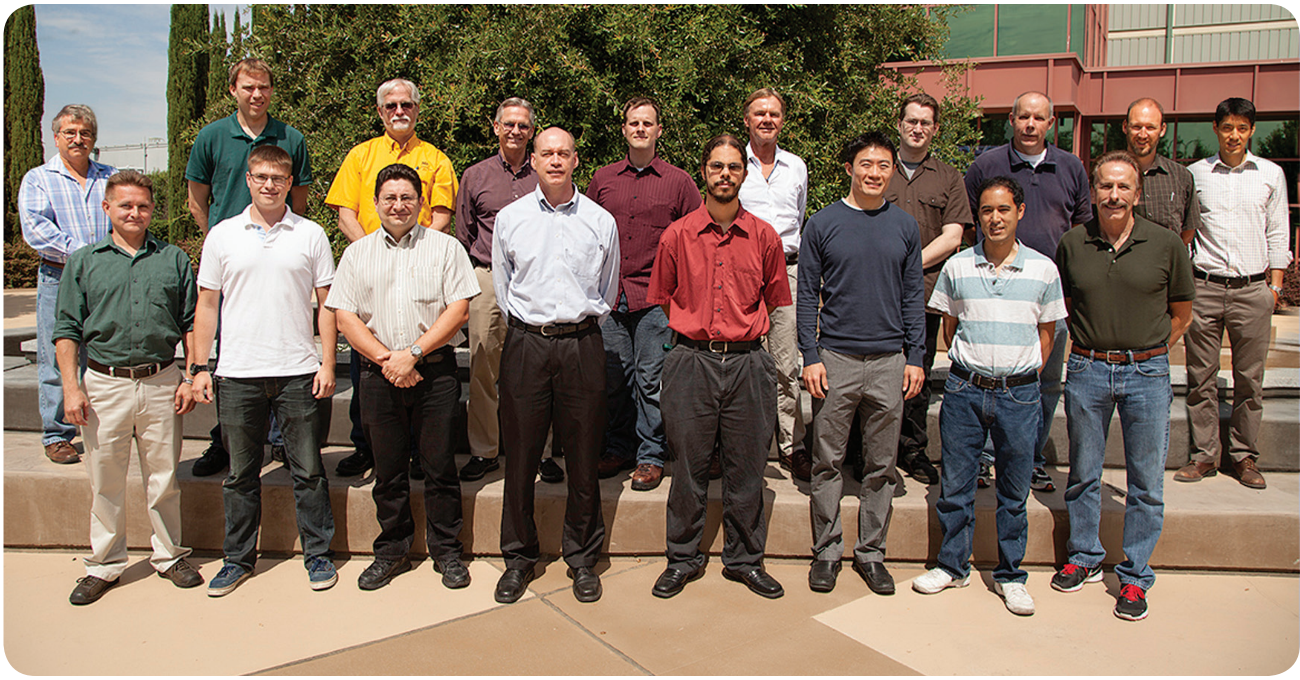
A Laboratory team led by optical engineer Jason Chou has developed an R&D 100 Award–winning technology, called Laser SHIELD (screening at high-throughput to identify energetic laser distortion), that identifies nonconforming pulses using a real-time 34-gigahertz oscilloscope. The new process not only reduces pulse-screening time from 12 hours or more to less than a second but also allows for greater operating efficiencies, eases system modifications, enables the laser to handle higher powers, and reduces operating costs.

The Danger of Powerful Beams

High-energy laser facilities such as NIF have become modern workhorses for scientific discovery in such disciplines as astrophysics, materials science, nuclear science, and particle physics. NIF is a critical experimental tool for the National Nuclear Security Administration's mission to ensure the continued safety, security, and reliability of the nation's nuclear weapons stockpile.

At NIF, 192 intense laser pulses direct nearly 2 million joules of ultraviolet light onto a tiny spherical target, creating extreme pressures and temperatures found only in stars. These unprecedented conditions could soon unleash the potential of controlled fusion energy gain. Eventually, intense light pulses could safely generate electricity fueled by hydrogen, the most abundant element in the universe.

The beams of light at NIF and other high-energy lasers are so powerful that they must be "conditioned" with an invisible frequency modulation (FM) to protect the laser system's valuable optics from harmful acoustic waves and hot spots. Equally important, steps must be taken to ensure that FM does not convert into a large and fast ripple on the pulse shape called amplitude modulation (AM). This transformation can result from spectral profile changes that occur during adjustments to laser characteristics, such as operating wavelength and power, or after routine maintenance of optical components. If left undetected, AM

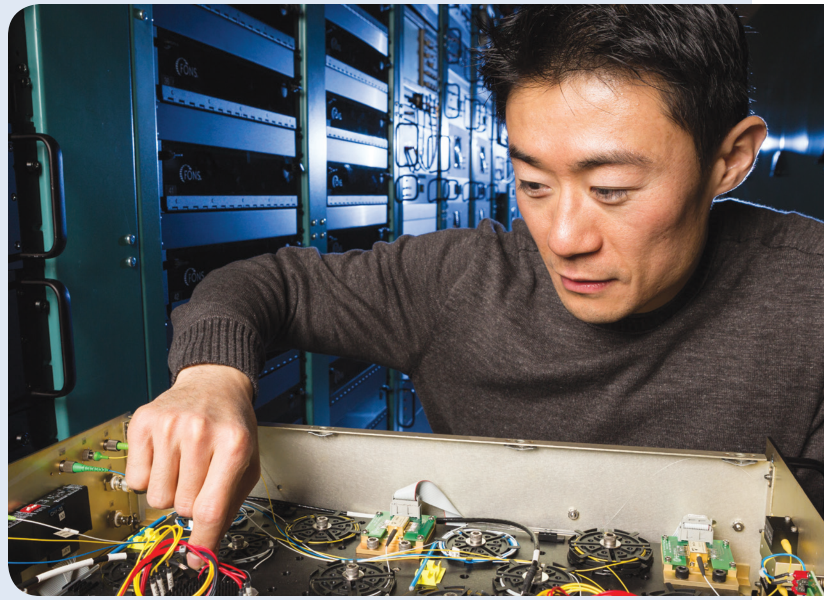


Development team for Laser SHIELD: (front row, from left) John Heebner, Alex Deland, Jean-Michel G. Di Nicola, Mark Bowers, Adrian Barnes, Jason Chou, Vincent Hernandez, and Don Browning; (back row) Anthony Rivera, Kevin Williams, Larry Smith, Gaylen Erbert, Jeff Jarboe, Kim Christensen, Matt Rever, Larry Pelz, Corey Bennett, and Leyen Chang.

on laser pulses may become harmful—exceeding safe levels near the target optics where pulse intensities are the strongest. AM must be periodically checked throughout the facility to ensure that laser pulses conform to safe operating conditions.

Prior to the development of Laser SHIELD, NIF operators used a manual process to screen for the presence of fast-pulse ripple at 48 checkpoints. The process required moving recording equipment from location to location throughout a facility the size of three football fields. In the past, NIF's operating conditions have been relatively static, requiring infrequent screening. Recently, however, NIF has transitioned into a more dynamic facility with added flexibility in power and wavelength. Much more frequent screening will be necessary to safeguard the laser.

"Today," says Chou, "the NIF team can monitor AM quickly and easily. The push of a button allows a single oscilloscope to simultaneously measure AM levels from 48 checkpoints throughout the NIF facility."



Livermore optical scientist Jason Chou looks over a new technology called Laser SHIELD (screening at high-throughput to identify energetic laser distortion). In the past, operators needed up to 12 hours to manually screen 48 critical checkpoints for harmful laser pulses at the National Ignition Facility. With Laser SHIELD, the screening can be done in less than 1 second and at the push of a button.

Laser SHIELD at Work

Laser SHIELD's high-throughput screening system is built entirely from low-cost, commercially available components found in the telecommunications industry. The all-fiber design makes it amenable to the unique needs of high-energy laser facilities. The fibers can be routed to intricate checkpoint locations, are immune to electromagnetic interference, and experience very low signal loss even over several kilometers.

The system operates in several steps. The initial step involves "freezing" the pulse shape as close as possible to each screening location. A wideband photodetector converts the light input into an electrical signal and then collects only AM data while rejecting the FM signal. As a result, FM–AM conversion no longer occurs in the new screening process.

Once the pulse shapes are in the electrical domain, they are imprinted onto a laser operating near 1,550 nanometers—a wavelength used by the telecommunications industry—using a radio-frequency amplifier to boost the signal. Next, optical fibers route pulses away from the checkpoints and ensure the 48 pulses do not overlap in time. When the pulses reach their final destination in the control room, a wavelength-division multiplexer combines them. A real-time wideband digitizer with up to 34-gigahertz bandwidth captures all locations in a 5-microsecond, single-shot acquisition. Raw data are processed to compute the AM result. Finally, a self-validation and calibration system ensures optimal performance and reliability over the life of the system.

At any time, a test pulse with predetermined AM can be created and distributed to all photodetectors as described in the initial step. The test pulse then undergoes the subsequent diagnostic steps, and the AM result is validated by comparing it with the predetermined AM setting. If discrepancies arise, an automatic calibration is performed and applied to the data-processing algorithm.

The team had explored other configurations, including fiber-optic lines at NIF's native wavelength and radio-frequency cabling running from the checkpoints to a single oscilloscope. But radio-frequency cabling involved signal loss, and fiber optics at other wavelengths could introduce distortion.

"Laser SHIELD is the first diagnostic of its kind capable of meeting the requirements of a high-energy laser facility," says Chou. The widespread presence of these laser research facilities throughout the U.S., Japan, China, France, and the United Kingdom is a testament to their invaluable role in research and development.

—Katie Walter

Key Words: high-energy laser pulse, Laser SHIELD (screening at high-throughput to identify energetic laser distortion), National Ignition Facility (NIF), R&D 100 Award.

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Mini-Apps Accelerate Hardware and Software Development

WHEN researchers and developers evaluate new high-performance computing (HPC) hardware approaches, especially radical departures from existing designs, a crucial step is selecting the right workloads to use in testing. During early stages of experimentation, they will often rely on small code fragments called kernels or benchmarking tools that offer streamlined deployment and data collection. Full-scale science and engineering applications, while the ultimate performance indicators, are often too large and complex to work with directly in early design studies. Thus, they are usually not executed until the final development stages, after the important design decisions are made. Unfortunately, kernels and benchmarking tools can be inadequate substitutes for real applications. In fact, as computer programs and platforms grow more complex, scientific application developers have noted a widening gap between benchmark results and how their codes perform on fully realized HPC systems.

Occupying a desirable middle ground between benchmarks and full-scale applications is a new category of compact, self-contained proxies for real applications called mini-apps. The mini-app concept was pioneered by the Mantevo Project, which is led by Michael Heroux and Richard Barrett of Sandia National Laboratories. Mantevo Project contributors include Livermore computational physicists David Richards and James Belak, as well as researchers from Los Alamos and Sandia national laboratories, NVIDIA Corporation, and three British institutions—the University of Bristol, the University of Warwick, and the Atomic Weapons Establishment. Mantevo Suite 1.0, the first integrated collection of mini-apps, has earned an R&D 100 Award.

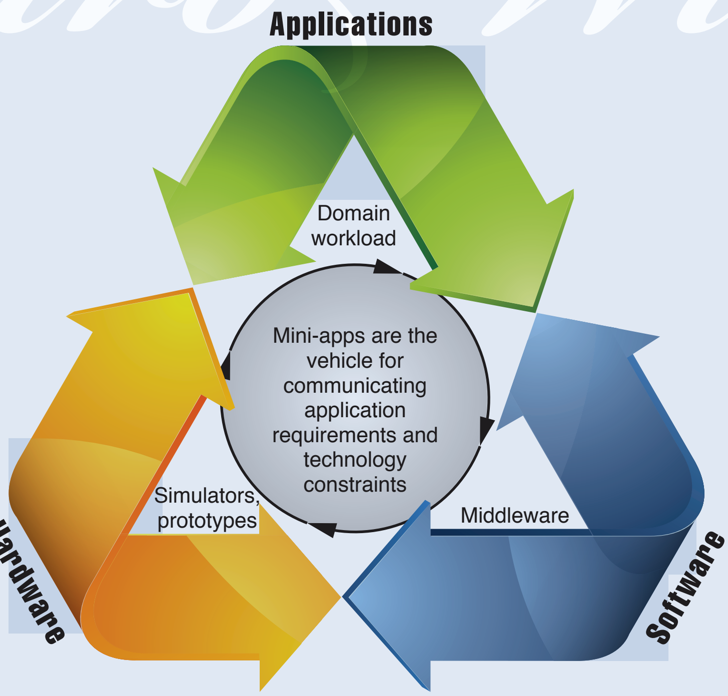
Livermore codevelopers of Mantevo Suite 1.0: (from left) James Belak and David Richards.

Identifying Performance Patterns

Mantevo mini-apps have quickly found a place in the HPC designer tool set because they can reliably predict application performance without the time, effort, and expertise that porting most full-scale codes to a new system would require. Averaging just 5,000 lines of code, the Mantevo mini-apps are comparatively easy to understand, deploy, modify, and even rewrite. As a consequence, they allow hardware developers to make earlier and better-informed design decisions, greatly improving the likelihood that the full-scale applications will perform successfully on the new system. Mini-apps are also useful for testing new programming models and languages, code compilation techniques, application scaling approaches, and other software-related experiments.

Mantevo Suite 1.0 contains miniature versions of seven HPC codes used for scientific and national security research. While many of the full-scale versions have access restrictions, the mini-apps are open-source software. Each mini-app is developed by the original application's code team, with the assistance of other experts. Although they are created independently and model different types of problems, all of the mini-apps share a common look and feel and are compatible with the suite's data collection and processing tools.

Mantevo mini-app developers strip a code of its nonessential elements and options and then focus on pattern identification. Although an application may have many modeling capabilities, the same underlying templates for data movement and processing



Application-driven co-design brings together vendors, hardware architects, system software developers, domain scientists, computer scientists, and applied mathematicians to make informed decisions about features and trade-offs in the design of high-performance computing hardware, software, applications, and underlying algorithms. Proxy applications, or mini-apps, help communicate the computational workload of full-scale applications as part of the co-design process.

will be repeated many times. By replicating only the essential patterns, the developers distill the essence of the full-sized program into a code a fraction of the program's size.

Livermore's contribution to the Mantevo Suite is the materials science proxy app Co-designed Molecular Dynamics (CoMD). Because CoMD contains most of the patterns in a full-sized classical MD code, it performs much the same. Furthermore, transformations that change how CoMD behaves will also apply to applications that share similar data patterns. Mantevo mini-apps such as CoMD are used regularly for performance design studies.

Predicting the Future by Inventing It

Computer scientists predict that the next generation of supercomputers will be notably different from previous generations. For the past two decades, hardware developers have produced faster computer microprocessors by increasing the speed and reducing the size of transistors, but transistors are nearing a lower limit in size and an upper limit in speed. Further speeding up the millions of transistors on a typical microprocessor would drive energy demands and operational costs for large-scale computing to untenable levels. (See *S&TR,* July/August 2013, pp. 4–13.) Going forward, performance gains will likely stem from redesigned processors that complete more computational tasks in parallel. Because the cost of data movement is also increasing, application developers are being asked to modify their algorithms. Instead of moving data to the compute processor, the computational work is being moved to the data.

These changes necessitate greater coordination between domain scientists, software developers, and hardware developers through an iterative and cooperative process called application-driven co-design. With application-driven co-design, scientific problem requirements influence computer architecture design, and system architecture technology constraints inform algorithm and software development. Lawrence Livermore researchers participate in several co-design projects funded by the Department of Energy (DOE), including the Exascale Co-design Center for Materials in Extreme Environments, a joint initiative with Los Alamos that has produced CoMD and various other mini-apps.

Mini-apps serve as a common language that researchers and developers can use to understand one another's needs and requirements during the co-design process. They expose hardware developers to simplified examples of codes that the scientific user community wants to execute on new systems. Because the tools are easily modified, both parties can alter them as part of design trade-off discussions and then quickly see how those changes affect performance. Lessons learned from the trade-off analyses are applied not only to the hardware designs but also to the full-scale application codes, thereby ensuring researchers can make the most of next-generation HPC hardware when it arrives.

Mini-apps provide a dynamic and increasingly popular platform for HPC testing and co-design activities. They have already aided the development of Livermore's Sequoia and Sandia's Cielo supercomputers and are an integral part of the co-design strategy for DOE's Extreme-Scale Computing Effort. Notes Richards, "Livermore has a long history of cooperation with hardware vendors, but mini-apps are taking it to a new level."

—*Rose Hansen*

Key Words: application-driven co-design, Co-designed Molecular Dynamics (CoMD), Extreme-Scale Computing Effort, Exascale Co-design Center for Materials in Extreme Environments, high-performance computing (HPC), Mantevo Suite 1.0, mini-app, R&D 100 Award, Sequoia.

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An Earthquake Exhibit with Magnitude

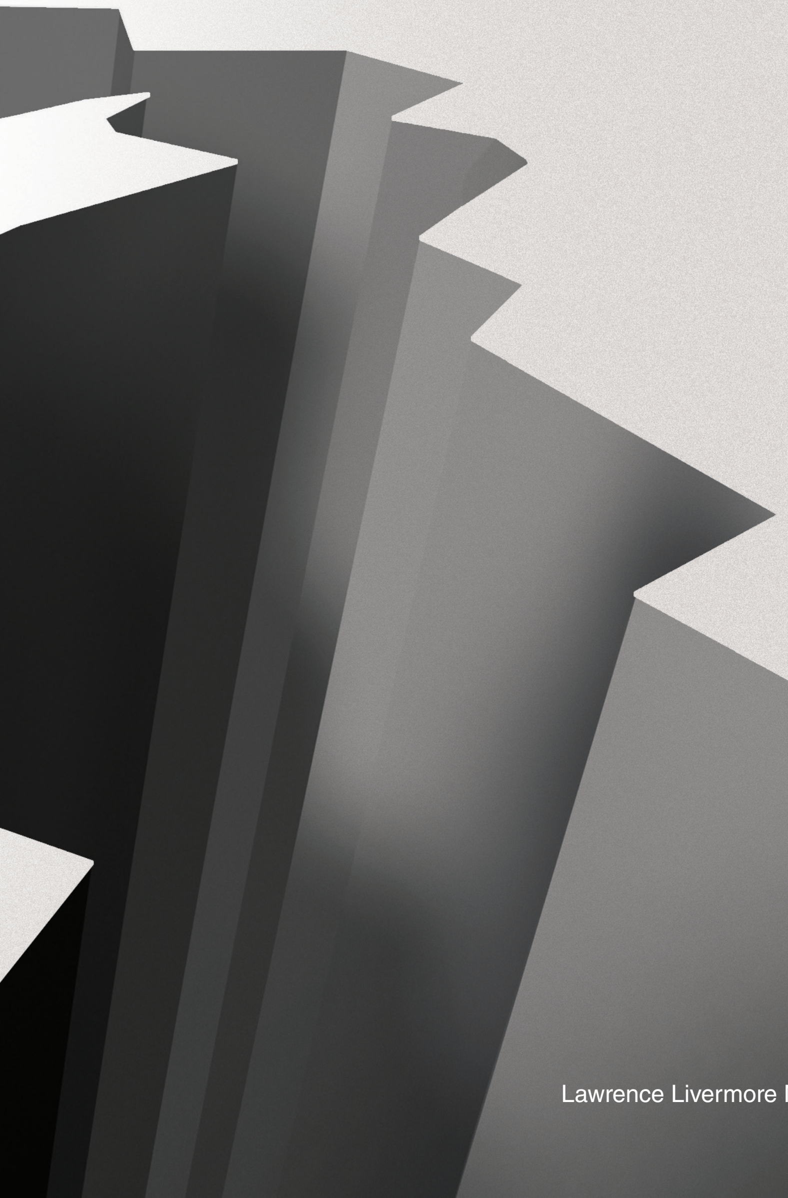
As residents of the nation's most seismically active state, most Californians view earthquakes with a mixture of fear and fascination. A major exhibit by the California Academy of Sciences in San Francisco, incorporating Lawrence Livermore simulation data, aims to replace the fear with understanding and even respect for how seismic forces shape the local and global landscape.

Creating an engaging yet scientifically accurate exhibit was the chief priority for the Academy's exhibition and visualization experts. "Earthquake: Evidence of a Restless Planet" was produced in collaboration with scientific and science education advisory panels and nearly 100 contributors from research institutions, including the U.S. Geological Survey (USGS), the University of California at Berkeley, and Lawrence Livermore. The core of the exhibit is a half-hour film presented in the Academy's Morrison

Planetarium, the world's largest all-digital full-dome theater. The film incorporates striking visualizations of earthquakes, tsunamis, and tectonic plate evolution. "Our all-digital planetarium has the capability of presenting complex topics—such as earth processes and the slow march of geologic time—within a very visual, immersive environment," says Ryan Wyatt, planetarium director and head of the Academy's visualization studio, where the film was developed.

One goal in making the film was to teach the public that scientists use not only field observations but also models and simulation to understand Earth's behavior. The scientific filmmakers were eager to showcase real simulation data whenever possible. "Earthquake" features 20 visuals generated directly from scientific data, more than any previous Academy film. Some visualizations were drawn from Lawrence Livermore seismic research such as accurate ground-motion simulations for two major earthquakes (one historical and the other hypothetical), simulations of seismic waves traveling through Earth, and a temperature map of Earth's interior based on global seismic-wave imaging. Laboratory seismologist Arthur Rodgers led the Livermore "Earthquake" collaboration team, which included Christina Morency, Nathan Simmons, Anders Petersson, and Bjorn Sjogreen.

At the California Academy of Sciences' Morrison Planetarium, an immersive, 27-meter-diameter dome theater currently features an award-winning half-hour film on earthquakes that was produced using scientific data from an array of institutions, including Lawrence Livermore.

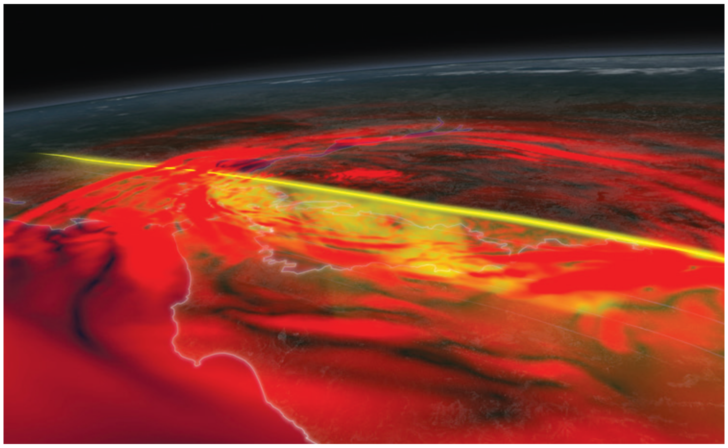


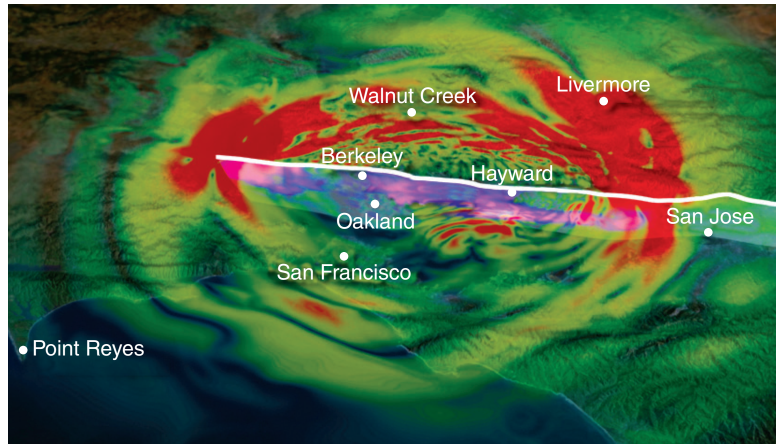
How to Draw an Earthquake

"When we started on the project," says Tom Kennedy, the film's producer, "we didn't realize the many different ways in which the data could be visualized. Through the input of the production team and focus groups, we found that some visualizations were misleading to people not versed in the dynamics of earthquakes, even though the visualizations made complete sense to scientists who were experts in the field." To avoid confusing or potentially alarming viewers, the filmmakers opted against showing an exaggerated distortion of ground velocity or displacement on a regional-scale map.

The Livermore team re-ran calculations from previous research efforts (see *S&TR,* September 2006, pp. 4–12), with some enhancements, to create even more accurate simulations that met the Academy's needs and scales. As an example, for regional-scale visualizations of San Francisco's 1906 magnitude 7.8 San Andreas Fault earthquake and a hypothetical magnitude 7.0 earthquake on the nearby Hayward Fault, the filmmakers and Livermore scientists focused on displaying two variables to which a general audience would relate—slip on the vertical fault plane and shaking intensity on Earth's surface. The Academy team used color intensity, rather than actual or exaggerated motion or displacement, which transformed the detailed simulation results into an intuitive and visually compelling animation. (See the figure on p. 16.)

Matt Blackwell, Academy studio technical director and data manager, says, "A key theme of the show is that an earthquake has many effects, from local to global, both on the surface and inside the planet. The Livermore team was able to





(left) A dome show visualization (courtesy of the California Academy of Sciences) of a hypothetical magnitude 7.0 earthquake along the Hayward Fault is derived from (right) a Livermore simulation of horizontal ground motion generated by Michael Loomis and Rich Cook. The Hayward Fault represents the highest hazard of all San Francisco Bay Area faults.

run simulations customized to our needs that show the 1906 San Francisco earthquake at many levels of detail and scales, with a continuous camera move from a local street view to a global level." A single shot early in the film, presenting the science behind the 1906 earthquake, integrates high-resolution photography, six simulations, and a historically accurate city model based on photographs, insurance maps, and personal accounts.

Supercomputer-Powered Seismology

Seismic-wave research is a core competency at Livermore. While most often associated with earthquakes, the research has many other applications of national interest, such as nuclear explosion monitoring, explosion forensics, energy exploration, and seismic acoustics. When studying seismic waves, Livermore scientists rely on two programs that run on powerful supercomputers—the Wave Propagation Program (WPP) for local- to regional-scale simulations and SPECFEM3D_GLOBE for global-scale simulations.

WPP uses three-dimensional models of the local geology and topography and the structure of the fault. Says Petersson, the program's creator, "WPP can work with any material model, of any size, as long as it fits on the computer." Because the speed of seismic waves largely depends on the rock types through which they travel, knowledge of regional geologic structure helps scientists determine when and how strongly a quake is felt at a given location. Regional-scale WPP simulations for the Academy collaboration, for instance, illustrate that even though the 1906 quake initially ruptured just west of San Francisco, surface-shaking intensity was highest some distance north of the city because of the amount of slip and the local geology.

SPECFEM3D_GLOBE, a code that accounts for Earth's spherical geometry and three-dimensional variations in seismic properties and topography, simulated ground motion and seismic-wave propagation during the 1906 earthquake on a larger scale. Researchers ran two calculations for the Academy project using this code—one for surface motion and one for seismic waves penetrating deep into Earth's interior. In the resulting visualization, filmmakers superimposed mantle temperature data provided by Simmons onto a slice of the interior wave simulation. Simmons used the Livermore-developed Earth model LLNL_G3D, which is an image of a large-scale geologic structure generated by analyzing the arrival times of millions of seismic waves passing through Earth. (See *S&TR*, March 2009, pp. 4–12.)

Displaying mantle temperature variations in the film helps illustrate another important point. Rodgers explains, "Earthquakes and other kinds of geologic activity are primarily caused by the motion of plates near the surface as they are pulled and pushed by mantle convection. These motions in the mantle are the result of heat trying to escape from Earth." (See the figure on p. 17.)

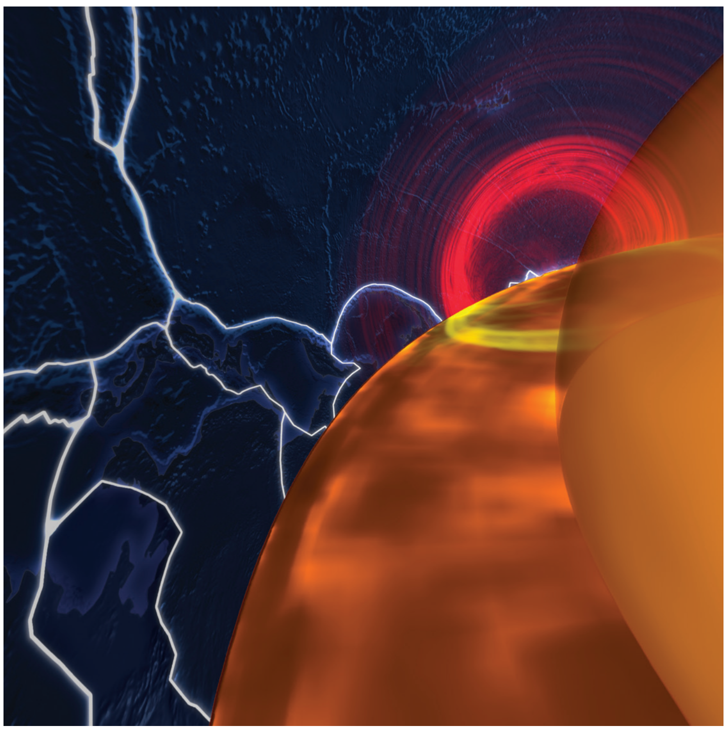
For the Academy effort, Livermore researchers simulated the San Andreas and Hayward fault events at high resolutions. Such calculations require significant computational resources. For the 1906 regional WPP simulation, for instance, simulating 125 seconds of ground motion required over 1 billion grid points, 10,000 time steps, and 7.5 hours of processor time on 2,048 cores of Livermore's Sierra machine. Thanks to refinements made over the past few years to a USGS three-dimensional subsurface model and to WPP, the simulation included for the first time the effects of realistic topography as well as geologic composition. This combination resulted in much more accurate estimates of ground motion on the area's hillsides and other susceptible areas. Eleven million velocity components on the surface are used to derive shaking-intensity information for each time step.

In the global SPECFEM3D_GLOBE calculation, the researchers had to split up the seismic-wave calculation for a one-sixth slice of Earth into several segments, because the full calculation generated data more quickly than Sierra's sizable parallel file system could handle. In total, simulations for the exhibit required over 30,000 computational hours on Laboratory supercomputers.

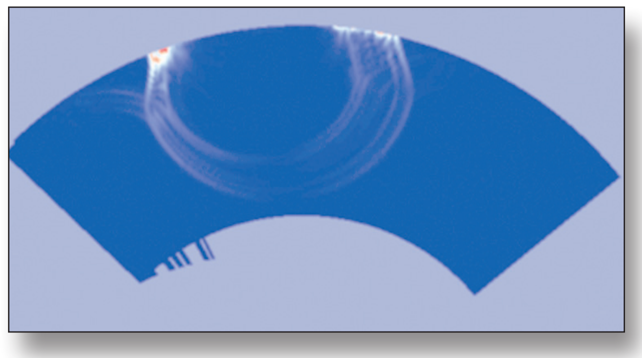
Making Waves with the Exhibit

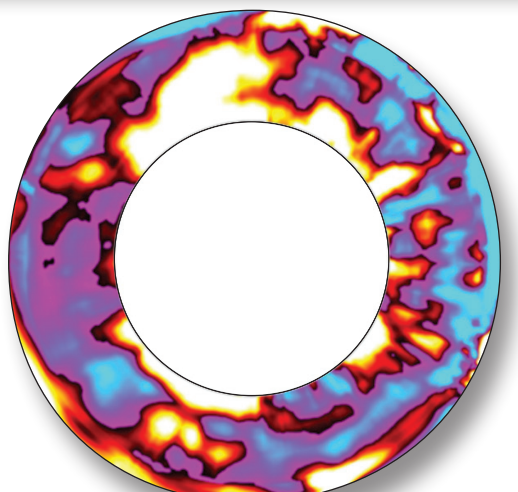
During the 17 months of film production, the Academy's visualization experts processed 175 terabytes (175 quadrillion bytes) of digital information; the Livermore contribution alone constituted gigabytes of data. The Laboratory exchanged data with the studio in a variety of formats, but the production team often worked directly with Livermore's raw data. The filmmakers used custom scripts to translate most of the data into a form compatible with the visual effects software Houdini.

Once in Houdini, the data were manipulated as needed and exported typically as a set of textures. These textures were mapped onto the fault plane, planetary surface, or other relevant geometry and rendered using the shot camera. Each step in the production process required close collaboration between the filmmakers and scientists to ensure scientific accuracy.



In the "Earthquake" show, a digital re-creation of San Francisco's 1906 earthquake incorporates a unique perspective of the event from within Earth, looking up at the surface (dark blue, with tectonic plate boundaries shown in white). The Academy's three-dimensional visualization illustrates seismic waves traveling along Earth's surface (red) and through the mantle below (yellow). The dark gold area is a cross section through the mantle along the San Andreas Fault, while the lighter gold region at far right is the core. (Visualization courtesy of the California Academy of Sciences.)





Incorporated into the Academy visualization at left is research by Livermore scientists such as (top) wave propagation calculations for a cross section through the mantle along the San Andreas Fault and (bottom) mantle temperature predictions.

Seismologist Arthur Rodgers (shown here) and other Livermore researchers also contributed to “Earthquake” interactive stations and educational displays.

Livermore contributions are also featured in the exhibit that accompanies the film and reinforces many of its themes. Visitors entering a 7.5-meter-high model of a slice of Earth (to scale) look up to see the mantle and core with the mantle textured using the same temperature data supplied for the planetarium show. Livermore seismic-wave calculations power an interactive screen displaying worldwide seismic activity. In addition, an earthquake simulator and stations on topics such as earthquake preparedness incorporate feedback from Livermore researchers.

The exhibit and film, which debuted in 2012, already have been seen by over half a million people, boosting the scientific literacy and earthquake preparedness of Bay Area residents and visitors alike. Audience response has been positive, and the film has received recognition for its outstanding special effects from the international Visual Effects Society. The Academy will feature “Earthquake” through 2014, and the film component will be licensed to other museums and planetaria worldwide; the studio’s previous in-house productions are currently showing at dome theaters in eight countries.

Through the efforts of Livermore animators Michael Loomis and Rich Cook, graphics and animations based on the same data sets now grace the Laboratory’s powerwalls and flat screens as well. The Livermore researchers are pleased to see their results transformed into stunning visuals and shared with a broad audience. Bill Goldstein, the Laboratory’s deputy director for Science and Technology, adds, “This partnership with the California Academy of Sciences allowed us to help educate and inform the public about the fascinating and important study of earthquakes, while showcasing the Lab’s unique contributions to the study of seismic activity.”

—Rose Hansen

Key Words: California Academy of Sciences, earthquake, LLNL_G3D, mantle tomography, seismic wave propagation, SPECFEM3D_GLOBE, Wave Propagation Program (WPP).

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Enterprise Modeling Leads to Smarter Decisions

THE nation's strategic deterrent, embodied in its arsenal of nuclear warheads, is supported and maintained by a sophisticated enterprise of laboratories, facilities, and people. Lawrence Livermore is a part of this enterprise and supplies key technologies and skills across the National Nuclear Security Administration (NNSA) complex. One particular Livermore product plays an integral role in supporting decision making: the Nuclear Weapons Enterprise Model. This model provides NNSA with a comprehensive view of the entire complex and enables better strategic decision making at the highest levels of management.

Designed by a team headed by Cliff Shang, a physicist in Livermore's Weapons and Complex Integration Directorate, the Nuclear Weapons Enterprise Model comprises a comprehensive database coupled to dynamic stockpile, infrastructure, and workforce models. The enterprise data include information about NNSA's assets, including its buildings, personnel, and the weapons themselves.

NNSA looks to enterprise modeling to project the effects of proposed reductions to the U.S. stockpile, the impacts of facility construction schedules, and the number of scientists and engineers needed to execute life-extension programs (LEPs) for nuclear weapons over the next decade. Shang says, "Enterprise models are ideal for testing implementation strategies, discovering inconsistencies, and identifying possible unanticipated consequences to policy options."

The complex has many aging facilities, including critical buildings built in the 1940s and 1950s, that are acutely in need of either modernization or replacement. (See the figure on p. 20.) Many highly specialized employees with critical skills that can take 10 years to acquire are nearing retirement. In addition, existing weapons have been in the stockpile for many years longer than originally intended.

By streamlining and consolidating operations, NNSA has closed 40 percent of all nuclear testing and production sites. Also, staff within the complex has been reduced by more than 60 percent over the last few decades. However, reduction decisions are becoming more difficult. If NNSA decides to eliminate another facility, unintended consequences on the nation's ability to conduct LEPs may occur, and the number of people who possess the critical skills to conduct a particular kind of work may be affected.

Collecting and Mining the Data

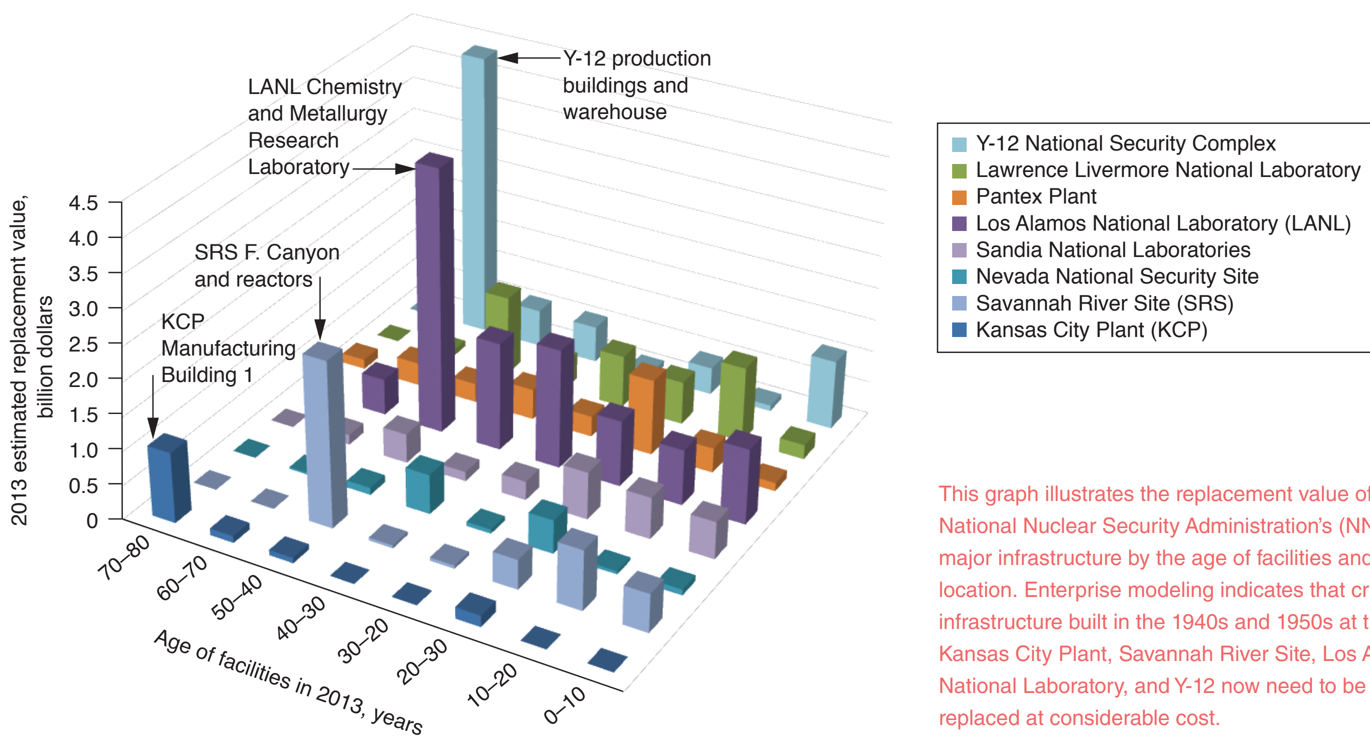
Since 2004, Livermore has worked closely with NNSA and its nuclear weapons laboratories and production plants to collect enterprise data, ensuring that the most current information is available for modeling calculations. A major challenge for code developers and analysts is to ensure the consistency of and to validate the detailed data gathered on NNSA's infrastructure, people, and stockpiled weapons. "The team conducts extensive verification and validation of modeling tools and data to ensure a comprehensive understanding of the range of applicability, sensitivity, and uncertainty in modeling results," says Shang.

The data come in many forms, and Livermore computer scientists Jeene Villanueva and Lisa Clowdus have written the code to structure the disparate information so that it can be correlated and connected with defined relationships. They have also built a user interface, which allows for rapid access to the validated, up-to-date enterprise data. Users can access information that ranges from a high-level view of the overall nuclear weapons complex to a specific detail about, for example, a ventilation or electrical system within a particular building. Villanueva says, "We collect enterprise-wide data and provide NNSA with the capability to access that data to perform stockpile life-cycle calculations, make infrastructure transformation choices, project the need for critical skills, evaluate data trends, and generate budget projections."

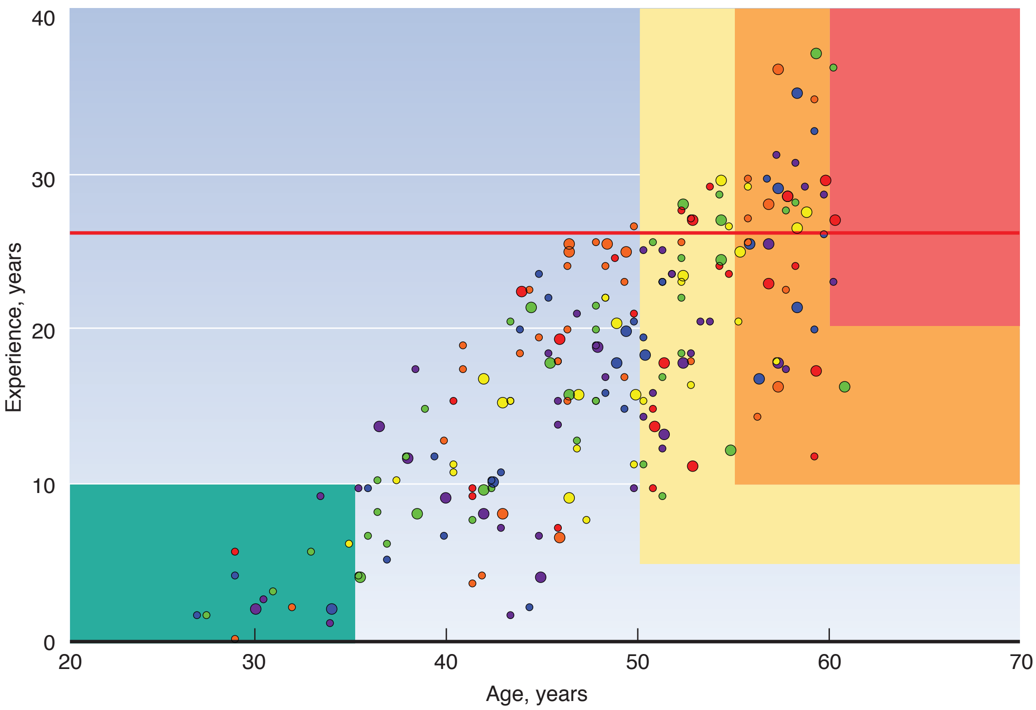
An Evolving Model

In its earliest incarnation, the model focused on NNSA's infrastructure and its employees with critical skills. (See *S&TR,* December 2005, pp. 4–10.) Using a systems dynamics approach, the model allowed NNSA to simulate proposed enterprise consolidation and streamlining. However, to make the nuclear weapons complex even smaller and less costly, NNSA needed even more information and model improvements. The enterprise model can now be used to evaluate the skills of the complex's entire workforce, all buildings and their components, and the stockpiled weapons. The model can also be used to evaluate plans to make the nuclear weapons complex safer and more secure.

Evolving to answer evermore difficult questions, the second-generation Livermore enterprise model incorporates mathematical techniques to provide simulation, optimization, economic-analysis, and decision-analysis tools. Shang explains, "In earlier versions of the model, as we were considering 'the big knobs' in the system, we developed codes in which a user entered input parameters to project an outcome. As we better understood the important variables in the enterprise model, we focused on implementing optimization models from the field of operations research."



This graph illustrates the replacement value of the National Nuclear Security Administration's (NNSA's) major infrastructure by the age of facilities and location. Enterprise modeling indicates that critical infrastructure built in the 1940s and 1950s at the Kansas City Plant, Savannah River Site, Los Alamos National Laboratory, and Y-12 now need to be replaced at considerable cost.



This chart depicts a projection of the critically skilled workforce in a specific NNSA program area in 2018. Each colored symbol represents a critical skill, which takes about 10 years to fully acquire. The bottom left shows employees entering the workforce as apprentices (green box), while the upper right shows experienced employees as they approach retirement age (yellow to orange to red). The red line indicates when nuclear tests were discontinued (1992). By 2018, essentially all of the workers who have had experience with conducting nuclear tests will be at or past retirement age.

With these tools, the enterprise model can simulate NNSA operations in detail and help assess how decisions would affect workflow. NNSA is able to evaluate different scenarios and examine how the enterprise model adjusts workflow to optimize results. Economic-analysis tools allow NNSA to estimate cost trajectories of stockpile, infrastructure, and science programs or campaigns. Finally, decision-analysis tools can be used to compare alternatives based on the preferences of decision makers.

In addition to merely projecting the effects of a proposed policy or the consequences of different budget scenarios, the enterprise model can now run through tens of thousands of decision variables to find the optimum solution and plot the best course of action. The model considers all the discrete entities that interact with each other. Probabilistic equations then provide potential best solutions and help eliminate poor decisions.

People as Enterprise Assets

Because the enterprise model includes detailed data about the entire workforce of the nuclear weapons complex, users can study statistics and trends such as how many people are employed; whether they work full or part time or as subcontractors; and what skills they possess. Users can also determine worker age distribution and years of experience, how much it costs to train personnel, and attrition rates. The model considers redundancy and is designed to optimize the workforce among the national laboratories and across the enterprise. It also allows NNSA to optimize workload to preserve and maintain critical skills.

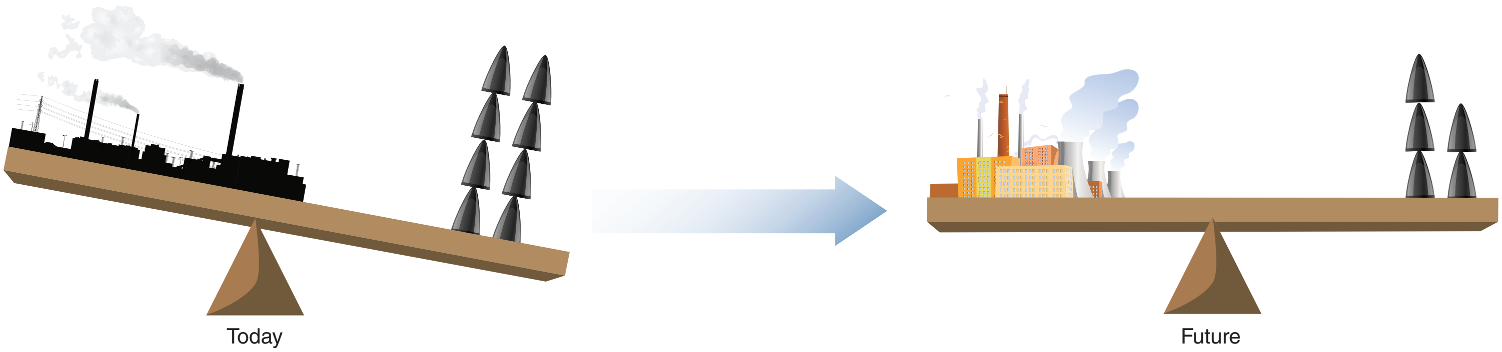
NNSA has long been concerned about recruiting and retaining personnel with critical skills for a modernized nuclear weapons complex. Over the last two decades, as NNSA has consolidated and closed facilities, the workforce has shrunk. In addition, employees with critical skills necessary for performing stockpile activities are retiring, and NNSA faces many challenges in replacing them. By 2018, essentially all of the workers who have had experience with conducting nuclear tests will be at or past retirement age.

As NNSA assesses staffing requirements for the coming years, it must determine what skills are needed and how those skills differ from historic needs. The challenge will be to fill positions for which there is a chronic shortage of qualified candidates who also have the training and capabilities in demand by high-technology firms in the private sector. Carol Meyers, a Livermore mathematician, says, “A major challenge for NNSA is ensuring that the new generation of weapons designers, code developers, experimentalists, stewards, and engineers are capable of developing a fundamental understanding of nuclear weapons in an environment where computer-aided design has taken the place of hands-on testing.”

By factoring in various scenarios, the model helps NNSA anticipate and cultivate the skills that will be needed for different projects, such as LEPs or increased dismantling of weapons. The model projects the optimal size staff for each location.

To Replace or Refurbish

Even though NNSA has closed 40 percent of its nuclear testing and production sites since the 1980s, future goals include reducing



Currently, the infrastructure of the nuclear weapons complex (which includes approximately 6,500 facilities with a capitalized value of about $40 billion) is outdated and has more than $900 million in deferred maintenance. If the nation prudently plans for a reduced future stockpile, old infrastructure can be replaced or modernized. Doing so would result in a U.S. nuclear weapons enterprise that is smaller, more balanced, safer, more secure, and less costly.

the total footprint of the complex even more, from 35 million to 26 million square feet. As the nuclear weapons complex continues to be consolidated, NNSA is placing greater emphasis on certain key facilities. Some of these facilities can be modernized and revitalized, while others will need to be replaced.

The model's optimization tools allow NNSA to illustrate how it can adroitly allocate a limited budget under a variety of scenarios. Users with access to detailed information about every building on the complex's eight sites can study a range of scenarios. For example, a major facility project may affect the flow of work throughout the entire complex, whereas a utility upgrade at a specific site may only interrupt operations temporarily but perhaps could impact an LEP schedule permanently.

The model can provide insight into the consequences of deferring maintenance, delaying the construction of a new facility, or even implementing a policy change. As expected, the model allows cost–benefit analysis of alternatives such as, for example, the trade-off between constructing a new facility versus sustaining and modernizing an existing facility. The entire life cycle of facilities from acquisition through mission use to demolition and decontamination are represented. Equally important, the model shows how infrastructure investments are tied to stockpile deliverables.

How Many Weapons Systems Are Optimal?

The Strategic Arms Reduction Treaty (START) and New START, which went into effect in 1994 and 2011, respectively, have limited the number of the nation's deployed strategic nuclear weapons. Meyers has developed a classified version of the enterprise model, called STORM (Stockpile Transformation Optimization Requirements Model), to help NNSA make stockpile decisions. Using STORM's simulation, optimization, economic-analysis, and decision-analysis tools, NNSA analysts can address questions about building, maintaining, and dismantling weapons systems based on the number of weapons, the length of their life cycle, their delivery system, the difficulty of maintaining them, and the complexity of an LEP. The model considers weapon dismantlement, which will be driven by stockpile reductions, as well as reuse and remanufacturing options.

For example, STORM is used in studies to minimize the number of years that warheads spend in the stockpile beyond their nominal service lifetimes. This objective is constrained by cost, the availability of people and facilities for work on the warheads, and the supporting infrastructure. The data and analyses support decisions about which weapons to maintain and which ones to dismantle. By evaluating different scenarios, NNSA can consider options to reduce the number of different types of weapons in the stockpile. For example, with fewer types of weapons, NNSA may be able to consolidate or eliminate some facilities.

The people, infrastructure, and weapons are the three major components of the nuclear weapons complex and are interdependent and linked by budget. Livermore's enterprise model helps NNSA to make fully informed decisions, with the knowledge that these decisions are soundly based on data. Because the model can evaluate options and look for optimal solutions, it helps ensure that NNSA understands the consequences when policies, budget, or other circumstances change. Shang and his team are working on a more complete model that combines both Department of Defense and NNSA assets, data, and plans, so that any decisions about the weapons can be closely coordinated with delivery systems.

—Karen Rath

Key Words: decision analysis, economic analysis, enterprise optimization, Nuclear Weapons Enterprise Model, simulation, Stockpile Transformation Optimization Requirements Model (STORM).

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Ultrawideband Radar Sensors and Networks

Richard R. Leach, Jr., Faranak Nekoogar, Peter C. Haugen
U.S. Patent 8,502,729 B2
August 6, 2013
Ultrawideband radar motion sensors strategically placed in an area of interest communicate with a wireless ad hoc network to provide remote area surveillance. Swept-range impulse radar and a heart and respiration monitor combined with a motion sensor further improves discrimination.

Spatially Adaptive Migration Tomography for Multistatic GPR Imaging

David W. Paglieroni, N. Reginald Beer
U.S. Patent 8,508,403 B2
August 13, 2013
This imaging and detection system is used to detect the presence of subsurface objects within a medium. In some embodiments, the imaging and detection system operates in a multistatic mode to collect radar return signals. An array of transceiver antenna pairs generates these signals. The array is positioned across the surface and travels down the surface. The imaging and detection system preprocesses the return signal to suppress certain undesirable effects. The system then generates synthetic aperture radar images from real aperture radar images generated from the preprocessed return signal. The system postprocesses the synthetic aperture radar images to improve the detection of subsurface objects. It also identifies peaks in the energy levels of the postprocessed image frame, which indicate the presence of a subsurface object.

Molten Salt Fuels with High Plutonium Solubility

Ralph W. Moir, Patrice E. A. Turchi, Henry F. Shaw, Larry Kaufman
U.S. Patent 8,506,855 B2
August 13, 2013
This invention includes a composition of lithium fluorine–thorium fluorine-4–uranium fluorine-4–plutonium fluorine-3 for use as a fuel in a nuclear engine.

Electro-Optic Device with Gap-Coupled Electrode

Robert J. Deri, Mark A. Rhodes, Andrew J. Bayramian, John A. Caird, Mark A. Henesian, Christopher A. Ebbers
U.S. Patent 8,514,475 B2
August 20, 2013
This electro-optic device has an electro-optic crystal with a predetermined thickness and first and second faces. A first electrode substrate is positioned opposite the first face. This first electrode substrate includes a first substrate material with a first thickness and a first electrode coating coupled to the first substrate material. A second electrode substrate is positioned opposite the second face. This second electrode substrate includes a second substrate material with a second thickness and a second electrode coating coupled to the second substrate material. A voltage source is electrically coupled to the first and second electrode coatings.

The Laboratory in the News *(continued from p. 2)*

Efficient Energy Harvesting Garners Journal Cover

Black metals could someday provide a pathway to more efficient photovoltaic solar cells to improve harvesting solar energy. A team of Livermore researchers led by engineer Tiziana Bond is experimenting with plasmonic black metals, which are nanostructured materials that have low reflectivity and high absorption rates of visible and infrared light. The nanopillar structures are trapping and absorbing sunlight. When black silicon, a semiconductor material, is roughened at the nanoscale level, it traps light by multiple reflections, increasing absorption to more efficiently trap the Sun's wavelengths. Team member physicist Mihail Bora reported this study in the cover article of the June 24, 2013, issue of *Applied Physics Letters*.

The plasmonic substrate studied by the researchers is composed of a square array of vertically coupled nanowires coated with gold, silver, or aluminum. The team's design is based on a cavity with multiple closely spaced resonances to form an oscillating system. The excitation end of the cavity is engineered to form an ultrasharp groove that broadens the plasmonic resonances and dissipates most of the incident energy into the metal, thus creating higher absorption rates.

The team's experiments have increased the average absorbance of the substrates to more than 75 percent above the visible range (400 to 800 nanometers). This achievement is remarkable considering all three metals are used to fabricate highly reflective optical mirrors. According to Bora, the significance of aluminum nanostructures for large-scale applications is underscored by the fact that aluminum is the least expensive pure metal and the third most abundant element in Earth's crust after oxygen and silicon. Coauthors include Elaine Behymer, Allan Chang, Keiko Munechika (now at Lawrence Berkeley National Laboratory), Dietrich Dehlinger (now at Illumina, Inc.), Cindy Larson, Hoang Nguyen, and Jerald Britten.

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Meteorite Mineral Named for Livermore Cosmochemist

A mineral discovered in a refractory inclusion of the Allende meteorite has been named in honor of Livermore cosmochemist Ian Hutcheon, who has made numerous contributions to the study of meteorites and what they reveal about the evolution of the early solar system. The discovery of the mineral by Sasha Krot from the University of Hawaii and Chi Ma from the California Institute of Technology was formally announced at the annual meeting of the Meteoritical Society in Edmonton, Canada, this past summer. The hutcheonite mineral structure and name have been officially approved by the International Mineralogical Association.

Refractory inclusions within meteorites are the oldest objects in the solar system. Hutcheon has been studying these, specifically in the meteorite Allende, since the 1970s, when he was a postdoctoral researcher at the University of Chicago. Allende is the largest carbonaceous chondrite meteorite ever found on Earth. It fell to the ground in 1969 over the Mexican state of Chihuahua and is notable for possessing abundant inclusions.

Hutcheon says, "I'm not in the business of discovering minerals, but I am interested in dating when these minerals formed and what happened to them several million years after they formed." Hutcheon is also interested in determining when water formed on the asteroid from which Allende and other carbonaceous chondrite meteorites originated. By looking at the concentrations of elements and isotopes in minerals found in the Allende inclusions, Hutcheon and his team can trace how water got there and ultimately how water developed in the early solar system. Hutcheonite, which is clear with a tinge of blue, is less than one-tenth the width of a human hair and can be seen only with high-powered scanning electron microscopes.

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Journal Cover Features Plutonium Cluster Study

Laboratory researchers Jim Tobin, Sung Woo Yu, and Brandon Chung, along with collaborators from the Russian Academy of Sciences and the E. I. Zababakhin Institute of Technical Physics, have developed a new approach to calculating the electronic structure of atomic clusters, specifically plutonium atom clusters. Their research appeared on the cover of the August 15, 2013, issue of *International Journal of Quantum Chemistry*.

For years, scientists have grappled with understanding how electronic structure changes as a function of the number of atoms in a cluster. "It has become clear over the past decade that an important mechanism for the long-distance transport of plutonium in groundwater is via suspended plutonium clusters or colloids," says Tobin. "The electronic structure of such clusters controls their reactivity with mineral surfaces and hence their transport characteristics."

The team's research combines theoretical results with spectroscopic data, confirming the validity of the approach. Many groups have worked toward understanding the electronic structure of solids as a function of system size. Progress on actinide-containing materials has been slowed by experimental limitations related to the highly radioactive and chemically toxic nature of these materials and by theoretical difficulties of correlated electron systems characteristic of high-atomic-number elements.

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Safety in the Skies

Livermore researchers are helping the federal government protect airlines from the threat of onboard explosives.

Also in December

• Computer simulations compare proposed methods for deflecting or disrupting an asteroid headed toward Earth.

• Scientists at the Center for Accelerator Mass Spectrometry apply bomb-pulse dating techniques to advance biological and forensics science research.

• Researchers are evaluating technologies to make renewable energy sources a powerful asset to electricity suppliers.

Coming Next Issue

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